TG07 **4:27 – 4:42**

THE NANOCOSMOS GAS CELL AS A TOOL FOR SPECTROSCOPY: THE MILLIMETERWAVE SPECTRUM OF N-ETHYLFORMAMIDE

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Several molecules containing a peptidic bond in their structure such as formamide ($HCONH_2$) and some derivative compounds have been already found in the interstellar medium[a]. In case of N-ethylformamide ($HCONHCH_2CH_3$), only the microwave spectrum is known up to 20 GHz hence the rotational constants for the conformers found are not accurate enough to detect the molecule in the interstellar medium.
In the present work we have employed the Nanocosmos Gas Cell spectrometer to record the millimeterwave spectrum of N-ethylformamide. The recently built broadband Fourier transform millimeterwave spectrometer[b] employs radio astronomical receivers for the Q-band (31.5-50GHz) and W-band (72-116GHz) to detect the thermal emission of the molecules in the Gas Cell chamber. The aim consists on establishing the concept of Nanocosmos Gas Cell as a new tool for high resolution broadband molecular spectroscopy in the millimeterwave region. In this study not only the ground state but also a higher energy conformer and some vibrational excited states have been identified and analyzed. The rotational constants will be used to search for this molecule in the space.

[a]R.H. Rubin *et al.*, **1971**, *ApJL*, 169, L39, and see *e.g.* A.J. Remijan *et al.*, **2014**, *ApJ*, 783, 77
[b]I. Tanarro *et al.*, **2018**, *A&A*, 609, A15 and J. Cernicharo *et al.*, **2019**, *A&A*

TG08 **4:45 – 5:00**

EXTENDED ANALYSIS OF THE ROTATIONAL SPECTRUM OF METHOXYISOCYANATE IN THE GROUND AND LOWEST EXCITED VIBRATIONAL STATES

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Methoxyisocyanate, CH_3ONCO is a methoxy derivative of isocyanic acid HNCO detected in the interstellar medium back in 1972[a]. Recent detections of methyl isocyanate, a methyl derivative of HNCO, towards Sgr B2(N)[b], and in the Orion[c], as well as the detection of methoxymethanol[d] motivated us to study the rotational spectrum of CH_3ONCO as a candidate molecule for searches in the interstellar medium. The previously presented study of the rotational spectrum of methoxyisocyanate[e] showed the complexity of the problem owing to the large amplitude motion, a skeletal torsion along ON bond. The analysis revealed the existence of the "ladder" Coriolis-type interactions between the ground and lowest skeletal torsional states. We present here the extension of the rotational spectrum analysis that includes new types of resonances as well as the assignment of new excited vibrational states of methoxyisocyanate. In particular, the inclusion of new resonances permitted to assign and fit within experimental accuracy high K_a transitions of the ground vibrational state.

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[a]Snyder, L.E. and Buhl, D. 1972, *ApJ*, **177**, 619
[b]Halfen, D.T., Ilyushin, V.V. and Ziurys, L.M. 2015, *ApJ*, **812**, L5
[c]Cernicharo, J. et al. 2016, *A&A*, **587**, L4
[d]McGuire, B.M. 2017, *ApJ* **851**, L46 (2017)
[e]Pienkina, A. et al. 2017, 72nd ISMS, WA03

TG09 **5:03 – 5:18**

FORMATION OF THE ALMA MOLECULE $HOCH_2CN$ AND RELATED SPECIES FROM THE REACTION OF C^+ WITH HCN AND HNC IN ICY GRAIN MANTLES

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Density functional theory cluster calculations indicate that the intermediate HOCHNC readily forms when C^+ reacts with HCN embedded in the surface of an icy grain mantle. Subsequent H addition to HOCHNC yields the iscyano compound $HOCH_2NC$. There is enough energy from the H addition for $HOCH_2NC$ to isomerize to $HOCH_2CN$ (glycolonitrile), an important prebiotic molecule that was recently detected with ALMA observations toward the solar-type protostellar source IRAS 16293-2422 B by Zeng et al. [MNRAS 2019, 484, L43]. It was found that H can also add to HOCHNC to form HOCHNCH without a barrier. The analogous reactions of C^+ with HNC in ice will also be discussed. Vibrational spectra of the various ice-bound reactants, intermediates, and products will be presented. The calculations were performed with B3LYP using aug-cc-pVDZ sets on C, N, and O and cc-pVDZ sets on H.